AMENDMENT TO THE CLAIMS

Kindly amend the claims, without prejudice, to read as follows:

Rewrite claim 1 to read as follows:

1. (Currently amended) A method for determining molecular crystal structures from powder diffraction data comprising the steps of:

providing a powder diffraction pattern of a molecular crystal structure;

generating a reduced representation of the powder diffraction pattern in dependence on a predetermined unit cell and space group of the molecule under examination in which the total quantity of diffraction data is significantly reduced whilst maintaining the characteristics of the diffraction data that are representative of the crystal structure under examination;

determining a set of variables for describing trial molecular structures, derived from predetermined internal coordinates and said space group;

assigning values to said variables thereby creating a population of trial structures each defined by a unique set of values for said variables;

calculating a fitness for each trial structure with respect to the reduced representation of the powder diffraction pattern;

determining whether any one of the calculated fitnesses is less than or equal to a predetermined threshold;

where none of the calculated fitnesses is less than or equal to the threshold value, selecting at least one survivor from the population of trial structures, altering the values of the variables of at least one of the survivors in accordance with one or more predetermined rules, calculating the fitnesses of the new trial structures; and repeating the steps of selecting survivors, altering the values of the variables and calculating the fitnesses of the new trial structures until at least one of the calculated fitnesses is less than or equal to the threshold value, and

where at least one of the calculated fitnesses is less than or equal to the threshold, outputting at least ~~on~~ one trial molecular crystal structure represented by the successful sets of values.

2. (Original) A method as claimed in claim 1, wherein the reduced representation includes single values representative of the intensity of each reflection in the powder diffraction data and one or more factors representative of the extent to which adjacent reflections overlap.

3. (Original) The method as claimed in claim 2, wherein the reduced representation consists of a structure factor intensity listing and associated covariance matrix.

4. (Previously Amended) The method as claimed in claim 2, wherein the total data in the reduced representation is reduced by a factor substantially equal to the number of data points in the original powder diffraction data divided by the number Bragg reflections in the measured data range.

5. (Previously Amended) The method as claimed in claim 3, wherein the fitness χ^2 of each of the trial structures is determined using the following function:

$$\chi^2 = \Sigma_h \Sigma_k \{(I_h - c \mid F_h \mid^2) (V^{-1})_{hk} (I_k - c \mid F_k \mid^2)\}$$

where:

$I_{h,k}$ = extracted intensity

$V_{h,k}$ = covariance matrix

c = a scale factor

$F_{h,k}$ = calculated structure factor from trial structure

6. (Previously Amended) The method as claimed in claim 1, wherein the set of variables consists of three coordinates representative of the location of the molecule within the unit cell and three independent coordinates representative of the orientation of the molecule within the unit cell.

7. (Original) The method as claimed in claim 6, wherein the set of variables includes one or more co-ordinates representative of variable torsion angles, bond angles or bond lengths.

8. (Previously Amended) The method as claimed in claim 1 including the step of determining the unit cell and space group for the molecule under examination.

9. (Previously Amended) The method as claimed in claim 1 including the step of determining the set of internal coordinates.

10. (Previously Amended) The method as claimed in claim 1, further including the step of monitoring the number of iterations in which new trial structures are generated and halting the method and outputting the trial crystal structure with the best calculated fitness after completion of a predetermined number of iterations.

11. (Previously Amended) The method as claimed in claim 1, wherein the selection of survivors and the alteration of the values of the variables is based on a simulated annealing procedure.

12-20. (Canceled)